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THE ELLIPSOIDAL VELOCITY DISTRIBUTION FUNCTION

by N. Stankiewicz

*Lewis Research Center
Cleveland, Ohio*

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ABSTRACT

An ellipsoidal velocity distribution function is found as the result of maximizing the entropy with constraints on the number density, the mean velocity, and the stress energy tensor. The relation of this function to the macroscopic flow equations (continuity, momentum, etc.) is studied. The special case of one-dimensional channel flow is analyzed. It is shown that the ellipsoidal distribution function gives a consistent description of viscous flow. That is, the parabolic flow profile and Newton's law of viscosity become natural consequences of the macroscopic flow equations.

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SUMMARY

An ellipsoidal velocity distribution function is found as the result of maximizing the entropy with constraints on the number density, the mean velocity, and the stress energy tensor. The relation of this function to the macroscopic flow equations (continuity, momentum, etc.) is studied. The special case of one-dimensional channel flow is analyzed. It is shown that the ellipsoidal distribution function gives a consistent description of viscous flow. That is, the parabolic flow profile and Newton's law of viscosity become natural consequences of the macroscopic flow equations.

INTRODUCTION

The concept of maximum entropy is well known in classical thermodynamics where it is used as a definition of the stable equilibrium condition. However, information theory, with its basic assumption that the disorder of a statistical system is a measure of its entropy, can provide a way of extending the maximum entropy concept to nonequilibrium situations.

The ellipsoidal velocity distribution function is an example of a nonequilibrium (non-Maxwellian) distribution function that can be derived from a maximum entropy (disorder) principle (ref. 1). Its name comes from the fact that the surfaces of constant density in velocity space are ellipsoids.

The derivation of the distribution function rests on the supposition that the entropy is a maximum, subject to various constraints. The constraints are those moments of the distribution function which, it is hypothesized, are deduced from measurements made on the system. They are all local averages and can change in time and with position. An open (flowing) system is considered.

The equations describing a flowing system are, in general, a hierarchy of equations involving the changes of a given moment of the distribution function in time; its transport

into and out of an infinitesimal volume; the changes because of external forces; and finally the irreversible changes caused by particle interactions.

This report is a study of the relation between the ellipsoidal distribution function and the macroscopic flow equations. The purpose herein is to show that the ellipsoidal distribution function gives a consistent description of viscous flow.

The procedure used in this report is in contrast to a previous work by this author (ref. 1) in which the relation between the Lagrange multipliers of different species within a single system (plasma) was investigated.

Holway (ref. 2) and Kogan (ref. 3) show that the distribution functions obtained by the Grad moment method are linearized expansions of the more general functions obtained by using the maximum entropy procedure. That is, those terms which depart from being Maxwellian are linearized in references 2 and 3. This implies that the departure from a Maxwellian distribution function and, hence, from equilibrium is small.

The present report takes the more general approach and leaves the distribution function intact. The relation of the ellipsoidal distribution function to the macroscopic flow equations is therefore not restricted to near-equilibrium or to related assumptions concerning the "binariness" of collisions.

ANALYSIS

Maximum Entropy

It is shown in reference 1 (and duplicated in appendix B of this report) that a displaced ellipsoidal velocity distribution function is the result of maximizing the entropy density

$$S = -\omega \left(\frac{m}{h}\right)^3 \int f(\ln f - 1) d^3 v \quad (1)$$

with the following moments of the distribution function as constraints:

Number density:

$$n = \omega \left(\frac{m}{h}\right)^3 \int f d^3 v \quad (2)$$

Mean velocity density:

$$n\langle \vec{v} \rangle = \omega \left(\frac{m}{h} \right)^3 \int f \vec{v} d^3 v \quad (3)$$

Stress-energy density tensor (per unit mass):

$$n\langle \vec{v} \vec{v} \rangle = \omega \left(\frac{m}{h} \right)^3 \int f \vec{v} \vec{v} d^3 v \quad (4)$$

(All symbols are defined in appendix A.) The nondimensional distribution function f is related to the density F of phase space by

$$F = \omega \left(\frac{m}{h} \right)^3 f \quad (5)$$

The moments defined by equations (2) to (4) are, by hypothesis (or by observation of the system), the independent variables of the system. That is, any other moment can be expressed in terms of these variables.

Taking a variation of S (the variation operates only on the distribution function) and introducing the constraints by means of the Lagrange multipliers $-\Omega$, $-\vec{\mu}$, and $-\hat{\vec{\Gamma}}$, we obtain (as shown in appendix B)

$$f = \exp(-\Omega - \vec{\mu} \cdot \vec{v} - \vec{v} \cdot \hat{\vec{\Gamma}} \cdot \vec{v}) \quad (6)$$

where

$$\vec{\mu} = -2\langle \vec{v} \rangle \cdot \hat{\vec{\Gamma}} \quad (7)$$

$$\hat{\vec{\Gamma}}^{-1} = 2(\langle \vec{v} \vec{v} \rangle - \langle \vec{v} \rangle \langle \vec{v} \rangle) \quad (8)$$

and

$$n = \omega \left(\frac{m}{h} \right)^3 \pi^{3/2} A^{-1/2} \exp(-\Omega + \langle \vec{v} \rangle \cdot \hat{\vec{\Gamma}} \cdot \langle \vec{v} \rangle) \quad (9)$$

where

$$A = \det \begin{bmatrix} \Gamma_{11} & \Gamma_{12} & \Gamma_{13} \\ \Gamma_{12} & \Gamma_{22} & \Gamma_{23} \\ \Gamma_{13} & \Gamma_{23} & \Gamma_{33} \end{bmatrix} \quad (10)$$

The specification of the distribution function consistent with the assumed information is complete. That is, all the Lagrange multipliers are given in terms of the independent moments of equations (2) to (4). Equations (7), (8), and (9) define $\vec{\mu}$, $\hat{\Gamma}$, and Ω , respectively, in terms of these moments.

The Ellipsoidal Distribution Function and the Hierarchy of Flow Equations

It is assumed in the preceding section that the constraints imposed by equations (2) to (4) are the results of measurements made on the system. However, these measured values may change in time, or from station to station within the system. There may also occur irreversible changes due to the internal interactions of particles.

The changes in the constraints can be found by taking the appropriate moments of the Boltzmann collision equation. Hence, corresponding to equations (2) to (4), for a system with no applied forces, the following equations can be derived:

$$\frac{\partial \rho}{\partial t} + \operatorname{div} \rho \langle \vec{v} \rangle = 0 \quad (11)$$

$$\frac{\partial \rho \langle \vec{v} \rangle}{\partial t} + \operatorname{div} \rho \langle \vec{v} \vec{v} \rangle = 0 \quad (12)$$

$$\frac{\partial \rho \langle \vec{v} \vec{v} \rangle}{\partial t} + \operatorname{div} \rho \langle \vec{v} \vec{v} \vec{v} \rangle = \left(\frac{\partial \rho \langle \vec{v} \vec{v} \rangle}{\partial t} \right)_I \quad (13)$$

where $\rho (=mn)$ is the mass density.

The left hand sides of these equations are the changes due to time and to transport, while the right hand sides contain the irreversibilities (sources and sinks) of the flows. Equations (11) and (12) are, therefore, expressions of conservation of mass and momen-

tum. The trace of equation (13) is the energy equation whose right hand side would include wall interactions. No use is made of this equation in this report.

An important point to notice about this set of equations is the occurrence of the next higher flow average - namely, $\rho\langle\vec{v}\vec{v}\vec{v}\rangle$. Also, the equation for $\rho\langle\vec{v}\vec{v}\vec{v}\rangle$ would contain $\rho\langle\vec{v}\vec{v}\vec{v}\vec{v}\vec{v}\rangle$. Seemingly a complete solution to any flow problem thus entails the solution of an infinite set of equations for all the flow averages. The usual resolution of this difficulty is to truncate arbitrarily the hierarchy of equations. The point of truncation usually coincides with the exhaustion of names for the higher terms - the heat flux generally being the last term considered.

The appearance of higher flow averages is not a problem if the distribution function is known, because the needed term is then calculable.

The maximum entropy technique outlined in the Maximum Entropy section (see p. 2) provides the most probable distribution function, consistent with the constraints considered. All higher moments are then calculable and expressable as functions of the independent constraining moments. This procedure is essentially an a priori truncation method for the set of equations (11), (12), and (13). From appendix B we get

$$\rho\langle v_i v_j v_k \rangle = \rho [\langle v_i \rangle \langle v_j v_k \rangle + \langle v_i v_j \rangle \langle v_k \rangle + \langle v_j \rangle \langle v_i v_k \rangle - 2\langle v_i \rangle \langle v_j \rangle \langle v_k \rangle] \quad (14)$$

Equation (14) is used in the next section to simplify equation (13) for analyzing a special case of viscous flow.

The Ellipsoidal Distribution Function and Viscous Flow

The purpose here is to show that the ellipsoidal distribution function gives a correct description of physical reality, in that it contains the elements of viscous flow.

The case considered is steady-state incompressible channel flow in which the flow velocity is one-dimensional in the x direction, that is,

$$\langle \vec{v} \rangle = \langle v_x \rangle \hat{\epsilon}_x \quad (15)$$

and the pressure tensor is

$$\hat{\mathbf{P}} = \rho [\langle \vec{v} \vec{v} \rangle - \langle \vec{v} \rangle \langle \vec{v} \rangle] = \begin{bmatrix} P & P_{wy} & 0 \\ P_{xy} & P & 0 \\ 0 & 0 & P \end{bmatrix} \quad (16)$$

where P is the scalar pressure.

Equations (11) and (15) with the conditions of steady-state and incompressible flow immediately specify that

$$\langle v_x \rangle = V(y) \quad (17)$$

Because of equations (15) and (11), equation (12) can be rewritten as

$$\operatorname{div} \rho (\langle \vec{v} \vec{v} \rangle - \langle \vec{v} \rangle \langle \vec{v} \rangle) = 0 \quad (18)$$

Then, with the use of equation (16), equation (18) becomes

$$\frac{\partial P}{\partial x} + \frac{\partial P_{xy}}{\partial y} = 0 \quad (19a)$$

$$\frac{\partial P}{\partial y} + \frac{\partial P_{xy}}{\partial x} = 0 \quad (19b)$$

It is assumed that the scalar pressure is constant in the y -direction, that is, transverse to the flow. Equation (19) then becomes

$$\frac{dP}{dx} + \frac{dP_{xy}}{dy} = 0 \quad (20)$$

where $P = P(x)$ and $P_{xy} = P_{xy}(y)$.

The final flow equation to be considered is equation (13), which expresses the changes in the stress-energy tensor but contains the higher moment $\rho \langle v_i v_j v_k \rangle$. Normally, this would be an unknown term, and for the analysis to continue, one would need to make some assumption concerning it. However, because of the maximum entropy procedure used in this report the most probable distribution function is known and this moment is calculable and given by equation (14).

Equation (13), with the use of (14), then reduces to

$$P \frac{dV}{dy} = \left(\frac{\partial P_{xy}}{\partial t} \right)_I \quad (21)$$

If the interaction term is linearized by

$$\left(\frac{\partial P_{xy}}{\partial t} \right)_I = -\nu P_{xy} \quad (22)$$

it is seen that equation (21) contains Newton's law of viscosity - namely,

$$P_{xy} = -\eta \frac{dV}{dy} \quad (23)$$

where $\eta = P/\nu$ is the coefficient of viscosity, and ν is an interaction frequency, or the reciprocal of a characteristic relaxation time.

Equations (20) and (23) can now be solved for the velocity profile. Each term in equation (20) must be equal to a constant so that for the case of constant viscosity equation (20) becomes

$$\frac{dp}{dx} = -K \quad (24a)$$

$$\frac{d^2V}{dy^2} = -\frac{K}{\eta} = -C \quad (24b)$$

where equation (23) was used in equation (24b). The scalar pressure, according to equation (24a), then varies linearly with the distance down the channel. And, solving equations (24), with the conditions

$$\left. \begin{array}{l} V = V_0 \quad \text{for} \quad \frac{dV}{dy} = 0, \quad y = 0 \\ V = 0 \quad \text{for} \quad y = \pm a \end{array} \right\} \quad (25)$$

yields the parabolic velocity profile

$$V = V_0 \left(1 - \frac{y^2}{a^2} \right) \quad (26)$$

It is thus seen that the ellipsoidal distribution function leads to a meaningful physical result.

CONCLUDING REMARKS

The principle of maximum entropy (disorder) consistent with the moments n , $n\langle \vec{v} \rangle$, and $n\langle \vec{v}\vec{v} \rangle$ as constraints leads to the ellipsoidal velocity distribution function. The constraints are introduced into a variational equation by means of Lagrange multipliers and these unknown multipliers are subsequently related to the constraints. The constraining moments are a set of independent macroscopic variables of the system.

In general, the flowing (open) system is described by a hierarchy of flow equations (continuity, momentum, etc.) which shows how the moments can vary with respect to position or time. However, the flow equations are not a closed set in that they always involve an unknown higher moment.

Because the constrained moments constitute an independent set of variables, the unknown moment is expressible in terms of the constraints. That is, all moments are calculable because the distribution function is known. Moreover, the distribution function is the most probable one consistent with the constraints considered. Thus, the principle of maximum disorder provides a consistent truncation for a given set of flow equations.

For the specific case of the ellipsoidal distribution function and for one-dimensional incompressible channel flow it is shown that the truncation of the flow equations contains Newton's law of viscosity. And this leads to a parabolic velocity profile.

An extension of the method to include heat flux and other higher moments is desirable and further studies might yield criteria predicting the point when higher moments must be introduced to describe adequately the flowing system in general.

Lewis Research Center,

National Aeronautics and Space Administration,

Cleveland, Ohio, November 12, 1968,

129-02-08-05-22.

APPENDIX A

SYMBOLS

A	determinant of the Γ matrix, defined in eq. (10)
c	constant
F	density in velocity-position (6-dimensional) space
f	velocity distribution function
h	Planck's constant
$\hat{\mathbf{I}}$	unit tensor
J	Jacobian, determinant of transformation matrix
K	constant
m	mass
n	number density
p	scalar pressure; or, with subscripts, component of pressure tensor
$\hat{\mathbf{P}}$	pressure tensor
S	entropy
V	mean velocity
$\vec{v}; (v_x, v_y, v_z)$	velocity vector; components
\vec{w}	velocity vector defined in eq. (B15)
(x, y, z)	components of position vector
β	parameter defined in eq. (B16)
$\hat{\Gamma}$	matrix of Lagrange multipliers
η	coefficient of viscosity
$\vec{\mu}$	vector whose components are Lagrange multipliers
γ	interaction frequency
$\vec{\xi}$	velocity vector defined in eq. (B12)
ρ	mass density
Ω	Lagrange multiplier
ω	degeneracy factor

Subscripts:

i, j, k running indices (= 1, 2, 3)

Mathematical symbols:

det determinant of

div divergence in coordinate space

grad gradient in coordinate space

grad_v gradient in velocity space

-1 inverse of

· dot or scalar product

→ vector

⊗ tensor symbol

⟨ ⟩ average value of

APPENDIX B

IDENTIFICATION OF THE LAGRANGE MULTIPLIERS

The variational equation used in deriving the ellipsoidal distribution function is

$$\delta S - \Omega \delta n - \vec{\mu} \cdot \delta(n \langle \vec{v} \rangle) - \hat{\vec{\Gamma}} \cdot \delta(n \langle \vec{v} \vec{v} \rangle) = 0 \quad (B1)$$

Substituting equations (1) to (4) into equation (B1) yields

$$-\omega \frac{m}{h}^3 \int \delta f (\ln f + \Omega + \vec{\mu} \cdot \vec{v} + \vec{v} \cdot \hat{\vec{\Gamma}} \cdot \vec{v}) d^3 v = 0 \quad (B2)$$

Because the variation δf is arbitrary, the integrand must vanish so that

$$f = e^{-\Omega - \vec{\mu} \cdot \vec{v} - \vec{v} \cdot \hat{\vec{\Gamma}} \cdot \vec{v}} \quad (B3)$$

which is the ellipsoidal distribution function in equation (6).

There are many ways to arrive at equation (7) and (8), but the simplest is as follows. Taking the gradient in velocity space of f gives

$$\text{grad}_v f = -f(\vec{\mu} + 2\vec{v} \cdot \hat{\vec{\Gamma}}) \quad (B4)$$

in which the symmetry of $\hat{\vec{\Gamma}}$ is used in equation (B4).

When integration is performed over all velocities, the left hand side of equation (B4) vanishes because f must vanish for infinite velocities:

$$\text{grad}_v f d^3 v = \sum_i \epsilon_i \int \frac{\partial f}{\partial v_i} dv_i d^2 v = \sum_i \epsilon_i \int [f(\infty) - f(-\infty)] d^2 v = 0$$

Hence, equation (B4) becomes

$$0 = -n \frac{1}{\omega} \left(\frac{h}{m} \right)^3 (\vec{\mu} + 2\langle \vec{v} \rangle \cdot \hat{\vec{\Gamma}}) \quad (B5)$$

where equations (2) and (3) were used. Finally,

$$\vec{\mu} = -2\langle \vec{v} \rangle \cdot \hat{\vec{\Gamma}} \quad (\text{B6})$$

which is equation (7) of the main text.

Substituting equation (B6) into equation (B4) and forming the diadic give

$$(\text{grad}_V f)\vec{v} = 2f\hat{\vec{\Gamma}} \cdot (\langle \vec{v} \rangle \vec{v} - \vec{v}\vec{v}) \quad (\text{B7})$$

and noticing that

$$\text{grad}_V(f\vec{v}) = \hat{\vec{I}}f + (\text{grad}_V f)\vec{v} \quad (\text{B8})$$

one arrives at

$$\text{grad}_V(f\vec{v}) - \hat{\vec{I}}f = 2f\hat{\vec{\Gamma}} \cdot (\langle \vec{v} \rangle \vec{v} - \vec{v}\vec{v}) \quad (\text{B9})$$

If equation (B9) is integrated over all velocities, the gradient term will again vanish. After simplifying one gets

$$\hat{\vec{I}} = 2\hat{\vec{\Gamma}} \cdot (\langle \vec{v}\vec{v} \rangle - \langle \vec{v} \rangle \langle \vec{v} \rangle) \quad (\text{B10})$$

Equation (B10) immediately defines equation (8); that is,

$$\hat{\vec{\Gamma}}^{-1} = 2(\langle \vec{v}\vec{v} \rangle - \langle \vec{v} \rangle \langle \vec{v} \rangle) \quad (\text{B11})$$

The integration of equation (2) to get the explicit form of n in equation (9) proceeds as follows. First, transform to the relative velocity variable $\vec{\xi}$, which is given by

$$\vec{v} = \langle \vec{v} \rangle + \vec{\xi} \quad (\text{B12})$$

From this it follows that

$$d^3 v = d^3 \xi \quad (\text{B13})$$

Then, with the use of equation (B6), the number density of particles in an incremental volume of velocity space $d^3 v$ becomes

$$\omega \left(\frac{m}{h}\right)^3 f d^3 v = \omega \left(\frac{m}{h}\right)^3 e^{-\Omega + \langle \vec{v} \rangle \cdot \hat{\vec{\Gamma}} \cdot \langle \vec{v} \rangle - \vec{\xi} \cdot \hat{\vec{\Gamma}} \cdot \vec{\xi}} d^3 \xi \quad (B14)$$

The easiest way to carry out the indicated integrals is to complete the square of each component (ξ_1, ξ_2, ξ_3). The following nonorthogonal transformation will accomplish this result:

$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix} = \begin{bmatrix} \Gamma_{11}^{1/2} & \frac{\Gamma_{12}}{\Gamma_{11}^{1/2}} & \frac{\Gamma_{13}}{\Gamma_{11}^{1/2}} \\ 0 & \left(\frac{\beta_{33}}{\Gamma_{11}}\right)^{1/2} & -\frac{\beta_{33}}{2 \Gamma_{11} \beta_{33}^{1/2}} \\ 0 & 0 & \left(\frac{A}{\beta_{33}}\right)^{1/2} \end{bmatrix} \begin{bmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{bmatrix} \quad (B15)$$

where

$$\left. \begin{aligned} \beta_{33} &= \Gamma_{11}\Gamma_{22} - \Gamma_{12}^2 \\ \beta_{23} &= 2(\Gamma_{12}\Gamma_{13} - \Gamma_{11}\Gamma_{23}) \\ A &= \det \hat{\Gamma} = \Gamma_{11}\Gamma_{22}\Gamma_{33} + 2\Gamma_{12}\Gamma_{13}\Gamma_{23}^2 - \Gamma_{11}\Gamma_{23}^2 - \Gamma_{22}\Gamma_{13} - \Gamma_{33}\Gamma_{12}^2 \end{aligned} \right\} \quad (B16)$$

It follows from equation (B15) that

$$\begin{aligned} d^3 w &= J d^3 \xi \\ &= A^{1/2} d^3 \xi \end{aligned} \quad (B17)$$

where J is the determinant of the transforming matrix in equation (B15). The integration in equation (B14) can now be carried out:

$$\begin{aligned}
n &= \omega \left(\frac{m}{h} \right)^3 A^{-1/2} e^{-\Omega + \langle \vec{v} \rangle \cdot \hat{\vec{\Gamma}} \cdot \langle \vec{v} \rangle} \int e^{-w^2} d^3 w \\
&= \omega \left(\frac{m}{h} \right)^3 \pi^{3/2} A^{-1/2} e^{-\Omega + \langle \vec{v} \rangle \cdot \hat{\vec{\Gamma}} \cdot \langle \vec{v} \rangle} \tag{B18}
\end{aligned}$$

which is equation (9).

Because of the independence of the Lagrange multipliers, one is able to compute any integral of f through a process of differentiation of n with respect to the Lagrange multipliers.

Therefore, note that

$$n = \int f d^3 v = n(\Omega, \vec{\mu}, \hat{\vec{\Gamma}}) \tag{B19}$$

and

$$\frac{\partial n}{\partial \mu_i} = - \int f v_i d^3 v = - n \langle v_i \rangle \tag{B20}$$

Likewise, since

$$\langle v_i \rangle = \frac{1}{n} \int f v_i d^3 v$$

then

$$\frac{\partial \langle v_i \rangle}{\partial \mu_k} = \frac{1}{n^2} \int f v_k d^3 v \int f v_i d^3 v - \frac{1}{n} \int f v_i v_k d^3 v = \langle v_k \rangle \langle v_i \rangle - \langle v_i v_k \rangle \tag{B21}$$

Lastly,

$$\langle v_i v_j \rangle = \frac{1}{n} \int f v_i v_j d^3 v$$

and

$$\frac{\partial \langle v_i v_j \rangle}{\partial \mu_k} = \langle v_i v_j \rangle \langle v_k \rangle - \langle v_i v_j v_k \rangle \quad (B22)$$

Equations (B22), (B21), and (B20) can now be rewritten in terms of first, second, and third order differentiations of n . If this is done, then equations (B20) and (B21) verify the results given by equations (B6) and (B11).

Equation (B22) is the defining equation for $\langle v_i v_j v_k \rangle$. Substituting equation (B11) yields

$$\begin{aligned} \langle v_i v_j v_k \rangle &= \langle v_i v_j \rangle \langle v_k \rangle - \frac{\partial \langle v_i v_j \rangle}{\partial \mu_k} \\ &= \langle v_i v_j \rangle \langle v_k \rangle - \frac{\partial}{\partial \mu_k} \left(\frac{1}{2} \Gamma_{ij}^{-1} + \langle v_i \rangle \langle v_j \rangle \right) \\ &= \langle v_i v_j \rangle \langle v_k \rangle - \langle v_i \rangle \frac{\partial \langle v_j \rangle}{\partial \mu_k} - \langle v_j \rangle \frac{\partial \langle v_i \rangle}{\partial \mu_k} \end{aligned} \quad (B23)$$

Now using equation (B21) gives

$$\langle v_i v_j v_k \rangle = \langle v_i v_j \rangle \langle v_k \rangle + \langle v_i v_k \rangle \langle v_j \rangle + \langle v_j v_k \rangle \langle v_i \rangle - 2 \langle v_i \rangle \langle v_j \rangle \langle v_k \rangle \quad (B24)$$

Multiplying equation (B24) by ρ then gives equation (14).

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